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Published in:
Acta Crystallographica Section E-Structure Reports Online

DOI:
[10.1107/S1600536806056479](https://doi.org/10.1107/S1600536806056479)

IMPORTANT NOTE: You are advised to consult the publisher's version (publisher's PDF) if you wish to cite from it. Please check the document version below.

Document Version
Publisher's PDF, also known as Version of record

Publication date:
2007

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Citation for published version (APA):

Muhammed, N., Zia-ur-Rehman, N. V., Ali, S., & Meetsma, A. (2007). 1,3-bis(4-bromophenyl)thiourea. *Acta Crystallographica Section E-Structure Reports Online*, 63, O632-O633.
<https://doi.org/10.1107/S1600536806056479>

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Key indicators

Single-crystal X-ray study

$T = 100$ K

Mean $\sigma(\text{C}-\text{C}) = 0.003$ Å

R factor = 0.028

wR factor = 0.072

Data-to-parameter ratio = 16.3

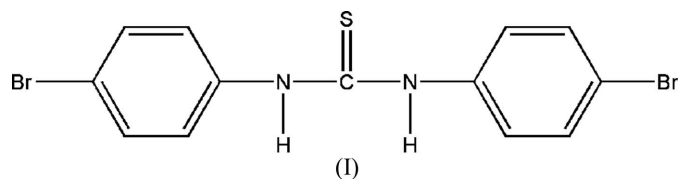
For details of how these key indicators were
automatically derived from the article, see
<http://journals.iucr.org/e>.

1,3-Bis(4-bromophenyl)thiourea

The two bromophenyl rings in the title compound, $\text{C}_{13}\text{H}_{10}\text{Br}_2\text{N}_2\text{S}$, adopt a *cis-cis* configuration to S with respect to the C—N thiourea bonds. The crystal packing is characterized by $\text{N}-\text{H}\cdots\text{S}$ hydrogen bonds.

Comment

N,N-disubstituted thiourea derivatives have attracted attention due to their coordination behavior with transition metals (Schuster *et al.*, 1990). Complexes with thiourea derivatives have also been investigated for their biological activities, such as antibacterial, antifungal, antitubercular, antithyroid and insecticidal activities (Madan & Taneja, 1991; Frech *et al.*, 1970).



The molecular structure of (I) is illustrated in Fig. 1. The short C—S distance [1.688 (2) Å] clearly shows its double-bond character. The two bromophenyl rings adopt a *cis-cis* configuration to S with respect to the C—N thiourea bonds, as observed in a homologous compound, (dichlorophenyl)thiourea (Soriano-Garcia *et al.*, 2001). The dihedral angles between the planes of the thiourea and the two bromophenyl rings (C1—C6, C8—C13) are 47.55 (10)° and 52.78 (10)°, respectively. A search of the distances yielded intermolecular contacts shorter than the sum of the van der Waals radii for N and S; the units are linked by hydrogen bonds (Steiner, 1996), forming an infinite one-dimensional chain along [010] (Table 1).

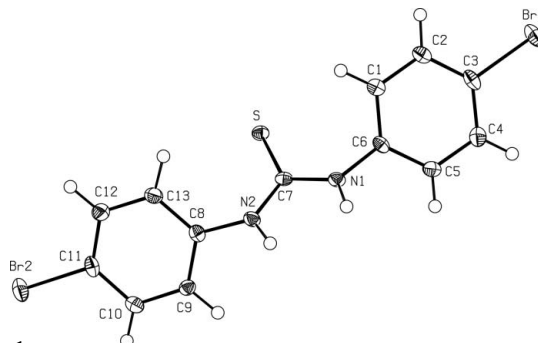


Figure 1

The molecular structure of the title compound. Displacement ellipsoids are drawn at the 50% probability level.

Experimental

A solution of 4-bromoaniline (1.72 g, 10 mmol) in acetone (20 ml) was added dropwise to a solution of CS₂ (0.90 ml, 10 mmol) and NH₃ (0.60 ml, 15 mmol) in acetone (20 ml). The mixture was stirred for about 4 h at room temperature. The solution was rotary-evaporated under vacuum. The crude product was then added to 10% HCl (200 ml) and stirred well. The solid product was separated off and recrystallized from dry acetone (yield 80%).

Crystal data

C ₁₃ H ₁₀ Br ₂ N ₂ S	Z = 4
<i>M_r</i> = 386.11	<i>D_x</i> = 1.887 Mg m ^{−3}
Monoclinic, <i>P</i> 2 ₁ / <i>c</i>	Mo <i>K</i> α radiation
<i>a</i> = 14.077 (1) Å	<i>μ</i> = 6.10 mm ^{−1}
<i>b</i> = 7.0804 (6) Å	<i>T</i> = 100 (1) K
<i>c</i> = 14.054 (1) Å	Block, colorless
<i>β</i> = 104.026 (1)°	0.46 × 0.42 × 0.37 mm
<i>V</i> = 1359.01 (18) Å ³	

Data collection

Bruker SMART APEX diffractometer	10894 measured reflections
<i>φ</i> and <i>ω</i> scans	3318 independent reflections
Absorption correction: multi-scan (<i>SADABS</i> ; Sheldrick, 2001)	2769 reflections with <i>I</i> > 2σ(<i>I</i>)
<i>T</i> _{min} = 0.073, <i>T</i> _{max} = 0.106	<i>R</i> _{int} = 0.029
	<i>θ</i> _{max} = 28.3°

Refinement

Refinement on <i>F</i> ²	$w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.2476P]$
$R[F^2 > 2\sigma(F^2)] = 0.028$	where $P = (F_o^2 + 2F_c^2)/3$
$wR(F^2) = 0.072$	(<i>Δ</i> / <i>σ</i>) _{max} = 0.001
<i>S</i> = 1.04	<i>Δρ</i> _{max} = 0.95 e Å ^{−3}
3318 reflections	<i>Δρ</i> _{min} = −0.42 e Å ^{−3}
203 parameters	
All H-atom parameters refined	

Table 1

Hydrogen-bond geometry (Å, °).

<i>D</i> —H··· <i>A</i>	<i>D</i> —H	H··· <i>A</i>	<i>D</i> ··· <i>A</i>	<i>D</i> —H··· <i>A</i>
N1—H21···S ⁱ	0.79 (2)	2.61 (2)	3.355 (2)	158 (2)
N2—H22···S ⁱ	0.79 (3)	2.53 (3)	3.316 (2)	168 (3)

Symmetry code: (i) $-x, y + \frac{1}{2}, -z + \frac{1}{2}$.

All the H atoms were located in a difference map, and all coordinates and isotropic displacement parameters were refined.

Data collection: *SMART* (Bruker, 2001); cell refinement: *SAINT-Plus* (Bruker, 2001); data reduction: *SAINT-Plus* and *XPREP* (Bruker, 2001); program(s) used to solve structure: *SIR2004* (Burla *et al.*, 2005); program(s) used to refine structure: *SHELXL97* (Sheldrick, 1997); molecular graphics: *PLATON* (Spek, 2003); software used to prepare material for publication: *PLATON*.

NM and Zia-ur-Rehman are grateful to the Higher Education Commission of Pakistan for financial support.

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supporting information

Acta Cryst. (2007). E63, o632–o633 [https://doi.org/10.1107/S1600536806056479]

1,3-Bis(4-bromophenyl)thiourea

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(I)

Crystal data

$C_{13}H_{10}Br_2N_2S$
 $M_r = 386.11$
 Monoclinic, $P2_1/c$
 Hall symbol: $-P\ 2ybc$
 $a = 14.077\ (1)\ \text{\AA}$
 $b = 7.0804\ (6)\ \text{\AA}$
 $c = 14.054\ (1)\ \text{\AA}$
 $\beta = 104.026\ (1)^\circ$
 $V = 1359.01\ (18)\ \text{\AA}^3$
 $Z = 4$
 $F(000) = 752$

The final unit cell was obtained from the xyz centroids of 5020 reflections after integration using the SAINTPLUS software package (Bruker, 2000).
 Reduced cell calculations did not indicate any higher metric lattice symmetry and examination of the final atomic coordinates of the structure did not yield extra symmetry elements (Spek, 1988; Le Page 1987, 1988)

$D_x = 1.887\ \text{Mg m}^{-3}$
 Mo $K\alpha$ radiation, $\lambda = 0.71073\ \text{\AA}$
 Cell parameters from 5020 reflections
 $\theta = 2.9\text{--}29.4^\circ$
 $\mu = 6.10\ \text{mm}^{-1}$
 $T = 100\ \text{K}$
 Block, colorless
 $0.46 \times 0.42 \times 0.37\ \text{mm}$

Data collection

Bruker SMART Apex
 diffractometer
 Radiation source: fine focus sealed Siemens Mo tube
 Parallel mounted graphite monochromator
 Detector resolution: $4096 \times 4096 / 62 \times 62$ (binned 512) pixels mm^{-1}
 φ and ω scans
 Absorption correction: multi-scan (SADABS; Sheldrick, 2001)

$T_{\min} = 0.073$, $T_{\max} = 0.106$
 10894 measured reflections
 3318 independent reflections
 2769 reflections with $I > 2\sigma(I)$
 $R_{\text{int}} = 0.029$
 $\theta_{\max} = 28.3^\circ$, $\theta_{\min} = 3.0^\circ$
 $h = -18 \rightarrow 18$
 $k = -9 \rightarrow 9$
 $l = -15 \rightarrow 18$

Refinement

Refinement on F^2
 Least-squares matrix: full
 $R[F^2 > 2\sigma(F^2)] = 0.028$
 $wR(F^2) = 0.072$
 $S = 1.04$
 3318 reflections
 203 parameters
 0 restraints
 Primary atom site location: heavy-atom method

Secondary atom site location: structure-invariant direct methods
 Hydrogen site location: difference Fourier map
 All H-atom parameters refined
 $w = 1/[\sigma^2(F_o^2) + (0.0404P)^2 + 0.2476P]$
 where $P = (F_o^2 + 2F_c^2)/3$
 $(\Delta/\sigma)_{\max} = 0.001$
 $\Delta\rho_{\max} = 0.95\ \text{e \AA}^{-3}$
 $\Delta\rho_{\min} = -0.42\ \text{e \AA}^{-3}$

Special details

Geometry. Bond distances, angles *etc.* have been calculated using the rounded fractional coordinates. All su's are estimated from the variances of the (full) variance-covariance matrix. The cell e.s.d.'s are taken into account in the estimation of distances, angles and torsion angles

Refinement. Refinement of F^2 against ALL reflections. The weighted R -factor wR and goodness of fit S are based on F^2 , conventional R -factors R are based on F , with F set to zero for negative F^2 . The threshold expression of $F^2 > \sigma(F^2)$ is used only for calculating R -factors(gt) *etc.* and is not relevant to the choice of reflections for refinement. R -factors based on F^2 are statistically about twice as large as those based on F , and R -factors based on ALL data will be even larger.

Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (\AA^2)

	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	−0.36823 (2)	0.19030 (3)	0.51761 (2)	0.0285 (1)
Br2	0.46781 (2)	0.19606 (3)	0.16394 (2)	0.0269 (1)
S	0.08535 (4)	0.15939 (7)	0.39401 (4)	0.0150 (1)
N1	−0.04879 (13)	0.4225 (3)	0.31854 (13)	0.0157 (5)
N2	0.09041 (13)	0.4346 (3)	0.26553 (13)	0.0165 (5)
C1	−0.09820 (16)	0.3287 (3)	0.46781 (17)	0.0168 (6)
C2	−0.17251 (16)	0.2784 (3)	0.51259 (18)	0.0185 (6)
C3	−0.26763 (16)	0.2620 (3)	0.45654 (18)	0.0190 (6)
C4	−0.29103 (17)	0.2971 (3)	0.35681 (18)	0.0205 (6)
C5	−0.21641 (16)	0.3469 (3)	0.31242 (17)	0.0175 (6)
C6	−0.12027 (15)	0.3619 (3)	0.36726 (16)	0.0149 (6)
C7	0.04089 (14)	0.3482 (3)	0.32398 (15)	0.0138 (6)
C8	0.18026 (14)	0.3759 (3)	0.24581 (16)	0.0157 (6)
C9	0.18244 (15)	0.3507 (3)	0.14874 (16)	0.0153 (5)
C10	0.26821 (16)	0.3002 (3)	0.12420 (18)	0.0181 (6)
C11	0.35179 (15)	0.2735 (3)	0.19824 (17)	0.0185 (6)
C12	0.35166 (17)	0.2991 (3)	0.29596 (18)	0.0207 (6)
C13	0.26545 (16)	0.3522 (3)	0.31977 (17)	0.0188 (6)
H1	−0.0312 (16)	0.340 (3)	0.5055 (17)	0.008 (5)*
H2	−0.1601 (18)	0.251 (3)	0.5822 (18)	0.017 (6)*
H4	−0.356 (2)	0.286 (3)	0.319 (2)	0.028 (7)*
H5	−0.2302 (16)	0.377 (3)	0.2480 (18)	0.015 (6)*
H9	0.1236 (17)	0.374 (3)	0.1001 (17)	0.015 (6)*
H10	0.272 (2)	0.287 (4)	0.060 (2)	0.027 (7)*
H12	0.411 (2)	0.285 (3)	0.346 (2)	0.026 (7)*
H13	0.2597 (17)	0.378 (3)	0.3902 (19)	0.022 (6)*
H21	−0.0697 (16)	0.492 (3)	0.2746 (18)	0.017 (6)*
H22	0.055 (2)	0.495 (4)	0.224 (2)	0.036 (8)*

Atomic displacement parameters (\AA^2)

	U^{11}	U^{22}	U^{33}	U^{12}	U^{13}	U^{23}
Br1	0.0248 (1)	0.0338 (2)	0.0324 (2)	−0.0052 (1)	0.0178 (1)	−0.0010 (1)
Br2	0.0177 (1)	0.0320 (1)	0.0337 (2)	0.0020 (1)	0.0117 (1)	−0.0026 (1)
S	0.0178 (2)	0.0136 (2)	0.0137 (3)	0.0010 (2)	0.0038 (2)	0.0013 (2)
N1	0.0190 (8)	0.0143 (8)	0.0146 (9)	0.0038 (7)	0.0058 (7)	0.0054 (7)

N2	0.0183 (8)	0.0165 (9)	0.0160 (10)	0.0027 (7)	0.0068 (7)	0.0046 (7)
C1	0.0208 (10)	0.0130 (9)	0.0174 (11)	−0.0002 (8)	0.0065 (9)	−0.0008 (8)
C2	0.0232 (11)	0.0163 (10)	0.0181 (12)	0.0006 (8)	0.0092 (9)	0.0001 (9)
C3	0.0210 (10)	0.0149 (9)	0.0257 (12)	−0.0003 (8)	0.0145 (9)	−0.0017 (9)
C4	0.0173 (10)	0.0212 (11)	0.0232 (12)	0.0006 (8)	0.0052 (9)	−0.0014 (9)
C5	0.0217 (10)	0.0165 (10)	0.0151 (11)	0.0027 (8)	0.0058 (9)	0.0011 (8)
C6	0.0186 (10)	0.0110 (9)	0.0176 (11)	0.0020 (8)	0.0094 (8)	−0.0009 (8)
C7	0.0184 (10)	0.0126 (9)	0.0102 (10)	−0.0016 (7)	0.0030 (8)	−0.0037 (7)
C8	0.0165 (9)	0.0128 (9)	0.0189 (11)	−0.0001 (8)	0.0065 (8)	0.0012 (8)
C9	0.0156 (9)	0.0148 (9)	0.0148 (10)	−0.0006 (8)	0.0022 (8)	0.0017 (8)
C10	0.0214 (10)	0.0178 (10)	0.0166 (12)	−0.0031 (8)	0.0077 (9)	−0.0016 (8)
C11	0.0144 (9)	0.0157 (10)	0.0274 (13)	−0.0012 (8)	0.0092 (9)	−0.0001 (9)
C12	0.0186 (10)	0.0249 (11)	0.0181 (12)	−0.0025 (8)	0.0034 (9)	0.0016 (9)
C13	0.0205 (10)	0.0209 (10)	0.0156 (11)	−0.0025 (8)	0.0055 (9)	0.0005 (9)

Geometric parameters (Å, °)

Br1—C3	1.895 (2)	C8—C13	1.394 (3)
Br2—C11	1.893 (2)	C8—C9	1.384 (3)
S—C7	1.688 (2)	C9—C10	1.381 (3)
N1—C6	1.414 (3)	C10—C11	1.382 (3)
N1—C7	1.353 (3)	C11—C12	1.386 (3)
N2—C7	1.346 (3)	C12—C13	1.387 (3)
N2—C8	1.421 (3)	C1—H1	0.97 (2)
N1—H21	0.79 (2)	C2—H2	0.97 (2)
N2—H22	0.79 (3)	C4—H4	0.94 (3)
C1—C6	1.391 (3)	C5—H5	0.90 (2)
C1—C2	1.392 (3)	C9—H9	0.95 (2)
C2—C3	1.384 (3)	C10—H10	0.92 (3)
C3—C4	1.382 (3)	C12—H12	0.96 (3)
C4—C5	1.391 (3)	C13—H13	1.03 (3)
C5—C6	1.390 (3)		
Br1···Br2 ⁱ	3.5362 (5)	C9···C4 ^{viii}	3.520 (3)
Br2···Br1 ⁱⁱ	3.5362 (5)	C9···C5 ^{viii}	3.570 (3)
Br2···C4 ⁱⁱⁱ	3.729 (2)	C10···S ^{ix}	3.625 (3)
Br2···C12 ^{iv}	3.739 (2)	C10···C3 ^{viii}	3.460 (3)
Br2···H4 ^v	2.95 (3)	C10···C4 ⁱⁱⁱ	3.581 (3)
S···C1	3.239 (2)	C10···C4 ^{viii}	3.537 (3)
S···C13	3.265 (2)	C10···C5 ⁱⁱⁱ	3.456 (3)
S···N2 ⁱⁱⁱ	3.316 (2)	C11···C5 ⁱⁱⁱ	3.555 (3)
S···C9 ^{vi}	3.510 (2)	C11···C4 ⁱⁱⁱ	3.520 (3)
S···N1 ⁱⁱⁱ	3.355 (2)	C12···Br2 ^x	3.739 (2)
S···C2 ^{vii}	3.472 (2)	C13···S	3.265 (2)
S···C10 ^{vi}	3.625 (3)	C1···H1 ^{xi}	2.94 (2)
S···H21 ⁱⁱⁱ	2.61 (2)	C7···H22 ⁱⁱⁱ	2.84 (3)
S···H22 ⁱⁱⁱ	2.53 (3)	C7···H1	2.97 (2)
S···H2 ^{vii}	3.08 (2)	C7···H13	3.00 (3)

S...H13	2.91 (2)	C7...H21 ⁱⁱⁱ	2.95 (2)
S...H1	2.83 (2)	H1...S	2.83 (2)
S...H9 ^{vi}	2.83 (2)	H1...C7	2.97 (2)
S...H10 ^{vi}	3.09 (3)	H1...C1 ^{xi}	2.94 (2)
N1...S ^{viii}	3.355 (2)	H1...H1 ^{xi}	2.45 (3)
N2...S ^{viii}	3.316 (2)	H2...S ^{vii}	3.08 (2)
C1...S	3.239 (2)	H4...Br2 ^{xii}	2.95 (3)
C2...S ^{vii}	3.472 (2)	H5...H21	2.35 (3)
C3...C10 ⁱⁱⁱ	3.460 (3)	H9...H22	2.35 (4)
C4...C11 ^{viii}	3.520 (3)	H9...S ^{ix}	2.83 (2)
C4...Br2 ^{viii}	3.729 (2)	H10...S ^{ix}	3.09 (3)
C4...C9 ⁱⁱⁱ	3.520 (3)	H13...S	2.91 (2)
C4...C10 ⁱⁱⁱ	3.537 (3)	H13...C7	3.00 (3)
C4...C10 ^{viii}	3.581 (3)	H21...H5	2.35 (3)
C5...C10 ^{viii}	3.456 (3)	H21...H22	2.05 (4)
C5...C8 ⁱⁱⁱ	3.500 (3)	H21...S ^{viii}	2.61 (2)
C5...C9 ⁱⁱⁱ	3.570 (3)	H21...C7 ^{viii}	2.95 (2)
C5...C11 ^{viii}	3.555 (3)	H22...H9	2.35 (4)
C6...C9 ^{viii}	3.564 (3)	H22...H21	2.05 (4)
C8...C5 ^{viii}	3.500 (3)	H22...S ^{viii}	2.53 (3)
C9...S ^{ix}	3.510 (2)	H22...C7 ^{viii}	2.84 (3)
C9...C6 ⁱⁱⁱ	3.564 (3)		
C6—N1—C7	128.21 (19)	C9—C10—C11	118.9 (2)
C7—N2—C8	127.1 (2)	Br2—C11—C10	118.53 (17)
C6—N1—H21	113.2 (17)	C10—C11—C12	121.5 (2)
C7—N1—H21	116.9 (17)	Br2—C11—C12	119.92 (17)
C7—N2—H22	112 (2)	C11—C12—C13	119.1 (2)
C8—N2—H22	116 (2)	C8—C13—C12	119.9 (2)
C2—C1—C6	119.7 (2)	C2—C1—H1	120.9 (14)
C1—C2—C3	119.6 (2)	C6—C1—H1	119.4 (14)
Br1—C3—C2	119.40 (18)	C1—C2—H2	122.4 (16)
Br1—C3—C4	119.14 (18)	C3—C2—H2	118.0 (15)
C2—C3—C4	121.5 (2)	C3—C4—H4	121.1 (17)
C3—C4—C5	118.7 (2)	C5—C4—H4	120.2 (17)
C4—C5—C6	120.7 (2)	C4—C5—H5	120.4 (15)
N1—C6—C1	122.2 (2)	C6—C5—H5	118.8 (15)
N1—C6—C5	117.79 (19)	C8—C9—H9	117.5 (15)
C1—C6—C5	119.9 (2)	C10—C9—H9	121.8 (15)
N1—C7—N2	113.76 (19)	C9—C10—H10	122.2 (18)
S—C7—N1	123.37 (16)	C11—C10—H10	118.9 (18)
S—C7—N2	122.82 (16)	C11—C12—H12	120.2 (16)
N2—C8—C13	122.4 (2)	C13—C12—H12	120.6 (16)
C9—C8—C13	119.9 (2)	C8—C13—H13	116.2 (14)
N2—C8—C9	117.62 (19)	C12—C13—H13	123.9 (14)
C8—C9—C10	120.6 (2)		
C7—N1—C6—C1	49.9 (3)	C2—C3—C4—C5	1.1 (3)

C7—N1—C6—C5	−134.1 (2)	C3—C4—C5—C6	−0.3 (3)
C6—N1—C7—S	0.0 (3)	C4—C5—C6—N1	−176.8 (2)
C6—N1—C7—N2	177.7 (2)	C4—C5—C6—C1	−0.6 (3)
C8—N2—C7—S	6.1 (3)	N2—C8—C9—C10	177.7 (2)
C8—N2—C7—N1	−171.7 (2)	C13—C8—C9—C10	0.7 (3)
C7—N2—C8—C9	124.7 (2)	N2—C8—C13—C12	−178.4 (2)
C7—N2—C8—C13	−58.4 (3)	C9—C8—C13—C12	−1.5 (3)
C6—C1—C2—C3	0.0 (3)	C8—C9—C10—C11	0.6 (3)
C2—C1—C6—N1	176.8 (2)	C9—C10—C11—Br2	177.91 (16)
C2—C1—C6—C5	0.8 (3)	C9—C10—C11—C12	−1.0 (3)
C1—C2—C3—Br1	179.19 (16)	Br2—C11—C12—C13	−178.72 (16)
C1—C2—C3—C4	−0.9 (3)	C10—C11—C12—C13	0.2 (3)
Br1—C3—C4—C5	−179.05 (16)	C11—C12—C13—C8	1.1 (3)

Symmetry codes: (i) $x-1, -y+1/2, z+1/2$; (ii) $x+1, -y+1/2, z-1/2$; (iii) $-x, y-1/2, -z+1/2$; (iv) $-x+1, y-1/2, -z+1/2$; (v) $x+1, y, z$; (vi) $x, -y+1/2, z+1/2$; (vii) $-x, -y, -z+1$; (viii) $-x, y+1/2, -z+1/2$; (ix) $x, -y+1/2, z-1/2$; (x) $-x+1, y+1/2, -z+1/2$; (xi) $-x, -y+1, -z+1$; (xii) $x-1, y, z$.

Hydrogen-bond geometry ($\text{\AA}, ^\circ$)

$D-H\cdots A$	$D-H$	$H\cdots A$	$D\cdots A$	$D-H\cdots A$
N1—H21 \cdots S ^{viii}	0.79 (2)	2.61 (2)	3.355 (2)	158 (2)
N2—H22 \cdots S ^{viii}	0.79 (3)	2.53 (3)	3.316 (2)	168 (3)
C1—H1 \cdots S	0.97 (2)	2.83 (2)	3.239 (2)	106.2 (15)
C9—H9 \cdots S ^{ix}	0.95 (2)	2.83 (2)	3.510 (2)	129.7 (18)

Symmetry codes: (viii) $-x, y+1/2, -z+1/2$; (ix) $x, -y+1/2, z-1/2$.